

OPTICAL SPECTRA AND MOLECULAR PARAMETERS OF LIGHT ELEMENT MOLECULES

By

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PROGRESS REPORT

I. Personnel

A. S. Kana'an, K. Sathianandan (not on contract funds),
and J. L. Margrave

II. Research Progress

The following research progress is to be reported:

(a) Vacuum Ultraviolet Spectroscopy

Due to a malfunction in the vacuum system of the two-meter McPherson spectrometer, Model 240, work on the spectrograph was interrupted temporarily before it was repaired by the McPherson Company.

Oxygen difluoride (OF_2) was excited in a hollow cathode discharge tube. No promising results were obtained in the visible and ultraviolet region. Work is continued in the vacuum ultraviolet region using various excitation devices.

A mixture of N_2 and Cl_2 was excited in a hollow cathode discharge tube and emission spectra were observed in the visible and ultraviolet regions. Preliminary studies did not indicate the presence of species of interest. The vacuum ultraviolet region will be investigated.

$(\text{BOF})_3$ was prepared and excited in a microwave discharge. The spectrum from this source is being investigated. A differential pumping system was attached to the spectrometer at the entrance slit to allow studies in windowless discharge tubes.

Absorption studies of various fluorides are planned.

(b) Visible and Near Ultraviolet Spectroscopy

Emission spectra from CF_4 , WF_6 , SiF_4 and H_2 introduced separately into the hot zone of the plasma were obtained. Preliminary studies showed successful mixing of these gases with the hot plasma. However, difficulties due to impurities in argon made it difficult to obtain spectra of CF , CF_2 , WF and H_2 molecules. The spectra of SiF and SiO were identified from the SiF_4 -Ar system. Spectra of CO and BO were identified in the case of CF_4 and WF_6 , respectively. An arrangement to inhibit interference of O_2 is under consideration.

(c) Infrared Spectroscopy

A special cell has been designed with cooling systems for work on the infrared spectrum of FeO_2 vapor. Also, several unsuccessful attempts were made to obtain the infrared spectrum of CrO_3 vapor. At elevated temperatures the substance decomposes to a series of lower oxides.

Infrared studies of SiF_2 (matrix) have been considered and a plan for getting SiF_2 deposited is being devised.

(d) Thermodynamic Properties of Light Element Molecules

Mass spectrometric studies of $NiF_2(g)$, $MnF_2(g)$ and $MnF(g)$ are in progress which will yield bond energies and heats of formation.

(e) Manuscripts and Meetings

1. A. S. Kana'an and J. L. Margrave, "Chemical Reactions in Electric Discharges," accepted for publication in Adv. Inorg. Chem. and Radiochemistry, Vol. 6 (1964).

2. A. S. Kana'an and J. L. Margrave, "Chemical Applications of Plasma Arc Devices," accepted for publication in Proc. Symp. on Plasma Arcs, World Metal Congress (1963).
3. K. Sathianandan, L. D. McCarty and J. L. Margrave, "Infrared Absorption Spectra of Inorganic Solids. III. Selenates and Selenites," accepted for publication, Spectrochimica Acta (1964).
4. C. P. Reguin, A. S. Kana'an and J. L. Margrave, "Plasma Chemistry," accepted for publication, Endeavor (1964).
5. K. Sathianandan and J. L. Margrave, "Molecular Constants of Some Nitrogen Fluorides," revision of manuscript in preparation.
6. A. S. Kana'an and J. L. Margrave, "Spectroscopic Investigations of Some Carbon and Silicon Halide Reactions in a Plasma Jet," manuscript in preparation.
7. K. Sathianandan, L. D. McCarty and J. L. Margrave, "Infrared Absorption Spectra of Inorganic Solids. IV. Hexafluorosilicates," manuscript in preparation.
8. K. Sathianandan and J. L. Margrave, "Infrared Spectra at High Temperatures. V. The Absorption Spectra of Selenium Dioxide Vapor," manuscript in preparation.
9. K. Sathianandan and J. L. Margrave, "Vibrational Spectra of $[(CF_3)_2CF]_2SiF_2$ and CF_3SiF_3 ," manuscript in preparation.